Nordic AI Meet 2026

O6. AI for Science & Engineering (Thu 12:30-13:30)

4. Structured Self-Driving Laboratory Automation of Chemical Synthesis via LLM- Generated XDL Protocol

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Abstract: Self-driving laboratories (SDLs) increasingly depend on autonomous robotic systems to carry out chemical procedures, but their adoption is still constrained by the need for expert programming and rigid workflow specifications. In this work, we present a Large Language Model (LLM)–driven framework that allows chemists to describe experimental tasks in natural language and automatically translates them into structured, machine-executable Chemical Description Language (XDL) protocols. The system incorporates a Retrieval-Augmented Generation (RAG) pipeline that grounds the LLM using XDL schema definitions, hardware capabilities, reagent metadata, and robotic skill descriptions, ensuring that the generated procedures remain aligned with laboratory constraints. An iterative error-detection and correction loop further validates and refines the XDL plans prior to execution. The resulting workflows are assessed in a simulation environment and demonstrated through a proof-of-concept deployment using a mobile manipulator operating across multiple laboratory workstations.